



## DFT-MRCI Hybrid Theory

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Many electronic structure problems are localised in the sense that the important electronic effects that influence a prediction can be viewed as occurring in a small region of space, or a subset of molecular orbitals. We split the overall orbital space of a system into two partitions,  $A$  and  $B$ , where  $A$  contains the chemically active orbitals. The spectator partition,  $B$ , is represented using an inexpensive low-level theory (eg. density functional theory (DFT)). At a cost comparable to that of using a high-level ab initio method, eg. multireference configuration interaction (MRCI), on  $A$  alone, we minimise an energy expression for the total system of the form,

$$E_{A\oplus B} = E_{A\oplus B}^{DFT} - E_A^{DFT} + E_A^{MRCI}.$$

The coupling between  $A$  and  $B$  arises properly through the variational minimization of the overall energy functional.